

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 15:19:17 ON 18 JAN 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:19:41 ON 18 JAN 2005

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STRUCTURE FILE UPDATES: 17 JAN 2005 HIGHEST RN 815574-28-8

DICTIONARY FILE UPDATES: 17 JAN 2005 HIGHEST RN 815574-28-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

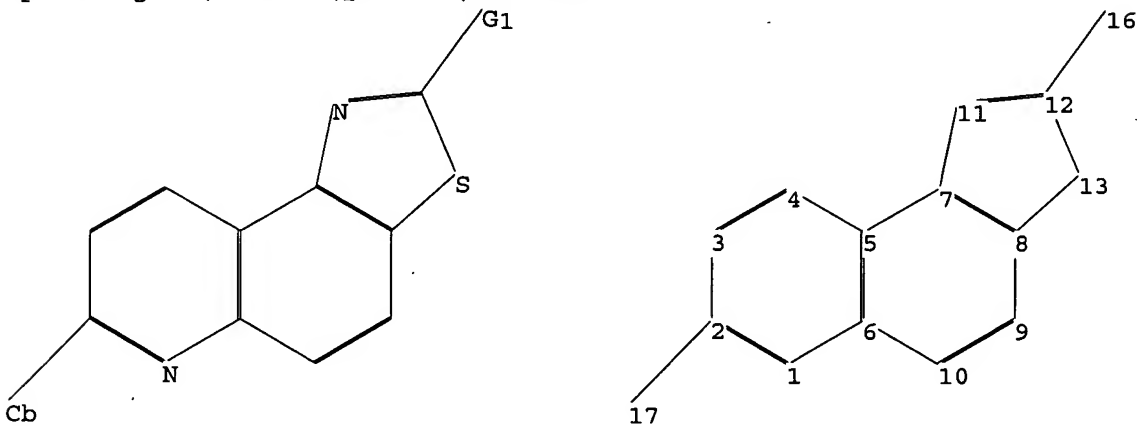
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\10-805860.str



chain nodes :

16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

2-17 12-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-13 9-10 11-12 12-13

exact/norm bonds :

7-11 11-12 12-16  
 exact bonds :  
 2-17 8-13 12-13  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10  
 isolated ring systems :  
 containing 1 :

G1:C,H

Match level :

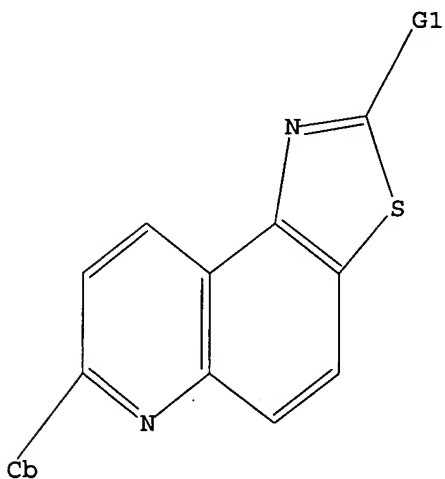
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 11:Atom 12:Atom 13:Atom 16:CLASS 17:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 15:19:57 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 622 TO ITERATE

100.0% PROCESSED 622 ITERATIONS

SEARCH TIME: 00.00.01

4 ANSWERS

L2 4 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE  
 ENTRY  
 161.33

TOTAL  
 SESSION  
 161.54

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:872797 CAPLUS

DOCUMENT NUMBER: 141:366224

TITLE: Tricyclic heteroaromatic compounds, particularly amino-substituted imidazoquinolines and thiazoloquinolines, with activity as N-type calcium channel blockers, and their preparation, pharmaceutical compositions, and use as analgesics

INVENTOR(S): Haeuel, Norbert; Draheim, Henning  
 PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany;  
 Boehringer Ingelheim Pharma GmbH & Co. KG

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

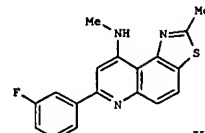
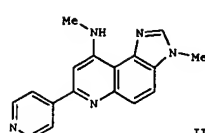
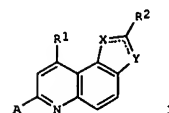
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089950	A1	20041021	WO 2004-EP3626	20040406
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SE, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10316659	A1	20041028	DE 2003-10316659	20030411
US 2004214833	A1	20041028	US 2004-805860	20040322
PRIORITY APPLN. INFO.:			DE 2003-10316659	A 20030411
			US 2003-465161P	P 20030424

OTHER SOURCE(S): MARPAT 141:366224

GI

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



AB The invention relates to tricyclic heteroarom. compds. I and salts thereof  
 [wherein: X = N, O, or S; Y = N when X = O or S; or Y = NR3, O, or S when X = N; A = (un)substituted mono-, di-, or tricyclic (hetero)aromatic with 0-3 N/O/S atoms, with at least one heteroatom being N; R1 = OH, F, Cl, Br, (di)alkylamino, (dicycloalkylamino, alkylcycloalkylamino, azetidin-1-yl, pyrrolidin-1-yl, pyrrolin-1-yl, imidazolidin-1-yl, imidazolin-1-yl, pyrazolidin-1-yl, pyrazolin-1-yl, piperidin-1-yl, piperazin-1-yl, morpholin-4-yl, thiomorpholin-4-yl, thiomorpholin-5-oxide-4-yl, thiomorpholin-5-dioxide-4-yl, or hexamethylenimino; R2, R3 = (independently) H, (cyclo)alkyl]. The invention further relates to the production of I and salts, and the use thereof as medicaments, in particular as analgesics. Ten compds. were prepared For instance, 3-oxo-3-(pyridin-4-yl)propionic acid Et ester was condensed with methylamine (as the acetate) (98t) to give an enamine, followed by amine exchange with 5-amino-1-methylbenzimidazole (26t), cyclocondensation to form the quinoline N-ring (82t), chlorination of the resultant phenolic hydroxy with POCl3 (23t), and aminolysis of the chloride with methylamine (17t), to give invention compound II. In a patch-clamp experiment involving recombinant HEK 293 cells expressing N-type calcium channels, invention compound III had an IC50 value of 2.0 µM.

IT 778624-10-5P, 9-(Dimethylamino)-7-(3-fluorophenyl)-2-methylthiazolo[4,5-f]quinoline 778624-12-7P, 7-(3-Fluorophenyl)-2-methyl-9-(methylamino)thiazolo[4,5-f]quinoline  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (drug candidate; preparation of amino-substituted imidazoquinolines and

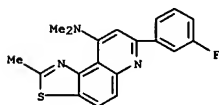
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

thiazoloquinolines as N-type calcium channel blockers for use as analgesics)

RN 778624-10-5 CAPLUS

CN Thiazolo[4,5-f]quinolin-9-amine, 7-(3-fluorophenyl)-N,N,2-trimethyl- (9CI)

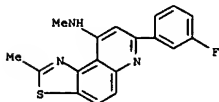
(CA INDEX NAME)



RN 778624-12-7 CAPLUS

CN Thiazolo[4,5-f]quinolin-9-amine, 7-(3-fluorophenyl)-N,2-dimethyl- (9CI)

(CA INDEX NAME)



IT 778624-21-8, 9-Chloro-7-(3-fluorophenyl)-2-methylthiazolo[4,5-f]quinoline

RL: RCT (Reactant); RACT (Reactant or reagent)

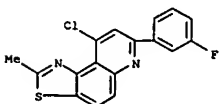
(starting material; preparation of amino-substituted imidazoquinolines and thiazoloquinolines as N-type calcium channel blockers for use as analgesics)

RN 778624-21-8 CAPLUS

CN Thiazolo[4,5-f]quinoline, 9-chloro-7-(3-fluorophenyl)-2-methyl- (9CI)

(CA

INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:5375 CAPLUS

DOCUMENT NUMBER: 78:5375

TITLE: Dyes of the condensed quinoline system

AUTHOR(S): Berni, E.

CORPORATE SOURCE: Ist. Chim. Org. Ind., Univ. Torino, Turin, Italy

SOURCE: Tinctoria (1972), 69(9), 309-14

CODEN: TINCAW; ISSN: 0040-7984

DOCUMENT TYPE: Journal

LANGUAGE: Italian

AB The relation of color and structure was determined from  $\lambda_{\text{maximum}}$  values for

a series of dyes based on thiazoloquinolines and thiadiazoloquinolines. NH<sub>2</sub>-substituted benzothiazoles and 1,2,3-benzothiadiazoles were condensed with MeCH:CHCHO and CH<sub>2</sub>:CHCO<sub>2</sub>Me, and quaternized with MeI to give I and II (X = CH, N; 7- or 9-Me). Styryl ( $\lambda_{\text{max}}$  529-597nm) and azamethine dyes ( $\lambda_{\text{max}}$  448-495nm) were prepared by condensing I and II with p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO and with XnC<sub>6</sub>H<sub>5</sub>-nN:NONa). Quinophthalone dyes ( $\lambda_{\text{max}}$  422-433nm) were also prepared by condensation of 7-methylthiazoloquinolines and 7-methylthiadiazoloquinolines with

phthalic

anhydride. The  $\lambda_{\text{maximum}}$  of azamethine and styryl dyes prepared from 9-methyl-substituted heterocycles were higher than those of dyes from the 7-methyl isomer; a bathochromic shift was also observed when the thiazole nucleus was replaced by thiadiazole. The azamethine  $\lambda_{\text{maximum}}$  was also influenced by the substituent(s) (X), increasing through the series X = 2,5-Cl<sub>2</sub>, 4-NO<sub>2</sub>, 2-MeO-4-NO<sub>2</sub>. The  $\lambda_{\text{maximum}}$  of the quinophthalones were slightly higher for those containing the thiadiazole nucleus. 2,6-Dimethyl-7,9-bis(p-(dimethylamino)styryl)selenazolo[5,4-f]quinolinium iodide, prepared by the same method as the other styryl dyes, exhibited 2 maximum between 500 and 600nm.

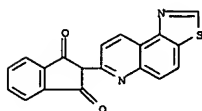
IT 40071-26-9

RL: PRP (Properties)

(visible spectrum of)

RN 40071-26-9 CAPLUS

CN 1H-Indene-1,3(2H)-dione, 2-thiazolo[4,5-f]quinolin-7-yl- (9CI) (CA INDEX NAME)



=&gt; fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

13.03

174.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.46

-1.46

FILE 'REGISTRY' ENTERED AT 15:24:00 ON 18 JAN 2005

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STRUCTURE FILE UPDATES: 17 JAN 2005 HIGHEST RN 815574-28-8

DICTIONARY FILE UPDATES: 17 JAN 2005 HIGHEST RN 815574-28-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

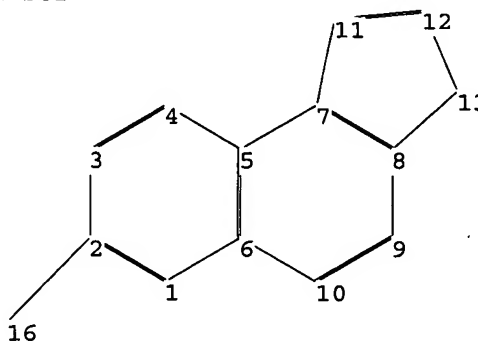
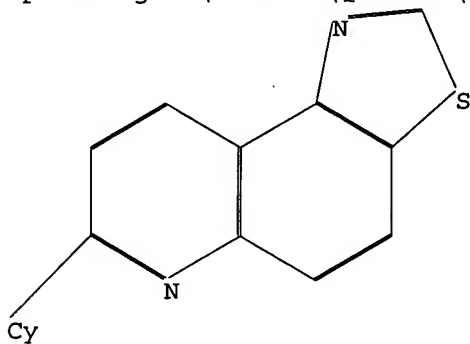
Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=&gt;

Uploading C:\STNEXP4\QUERIES\10-805860a.str



chain nodes :

16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

2-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-13 9-10 11-12 12-13

exact/norm bonds :

2-16 7-11 11-12  
 exact bonds :  
 8-13 12-13  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10  
 isolated ring systems :  
 containing 1 :

G1:C,H

Match level :

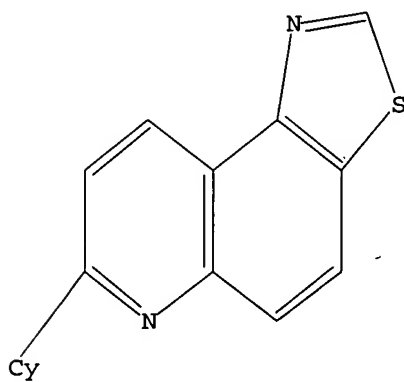
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 16:Atom

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s l4 ful

FULL SEARCH INITIATED 15:24:18 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 622 TO ITERATE

100.0% PROCESSED 622 ITERATIONS  
 SEARCH TIME: 00.00.01

7 ANSWERS

L5 7 SEA SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE  
 ENTRY  
 161.33

TOTAL  
 SESSION  
 335.90

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.46

FILE 'CAPLUS' ENTERED AT 15:24:20 ON 18 JAN 2005  
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FILE COVERS 1907 - 18 Jan 2005 VOL 142 ISS 4  
 FILE LAST UPDATED: 17 Jan 2005 (20050117/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l5

L6 2 L5

=> d his

(FILE 'HOME' ENTERED AT 15:19:17 ON 18 JAN 2005)

FILE 'REGISTRY' ENTERED AT 15:19:41 ON 18 JAN 2005

L1 STRUCTURE UPLOADED

L2 4 S L1 FUL

FILE 'CAPLUS' ENTERED AT 15:20:00 ON 18 JAN 2005

L3 2 S L2

FILE 'REGISTRY' ENTERED AT 15:24:00 ON 18 JAN 2005

L4 STRUCTURE UPLOADED

L5 7 S L4 FUL

FILE 'CAPLUS' ENTERED AT 15:24:20 ON 18 JAN 2005

L6 2 S L5

=> s l6 not l3

L7 0 L6 NOT L3

=> d ibib abs hitstr l6 2

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:5375 CAPLUS

DOCUMENT NUMBER: 78:5375

TITLE: Dyes of the condensed quinoline system

AUTHOR(S): Barni, E.

CORPORATE SOURCE: Ist. Chim. Org. Ind., Univ. Torino, Turin, Italy

SOURCE: Tinctoria (1972), 69(9), 309-14

CODEN: TINCAW; ISSN: 0040-7984

DOCUMENT TYPE: Journal

LANGUAGE: Italian

AB The relation of color and structure was determined from  $\lambda_{\text{maximum}}$  values for

a series of dyes based on thiazoloquinolines and thiadiazoloquinolines. NH<sub>2</sub>-substituted benzothiazoles and 1,2,3-benzothiadiazoles were condensed with MeCH:CHCHO and CH<sub>2</sub>:CHCOMe, and quaternized with MeI to give I and II (X = CH, N; 7-or 9-Me). Styryl ( $\lambda_{\text{max}}$  529-597nm) and azamethine dyes ( $\lambda_{\text{max}}$  448-495nm) were prepared by condensing I and II with p-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHO and with XnC<sub>6</sub>H<sub>5</sub>-nN:NONa). Quinophthalone dyes ( $\lambda_{\text{max}}$  422-433nm) were also prepared by condensation of 7-methylthiazoloquinolines and 7-methylthiadiazoloquinolines with

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IT 40071-26-9

RL: PRP (Properties)  
(visible spectrum of)

RN 40071-26-9 CAPLUS

CN 1H-Indene-1,3(2H)-dione, 2-thiazolo[4,5-f]quinolin-7-yl- (9CI) (CA INDEX NAME)

